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Tunneling quantum current in carbon nanotube's junctions

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Theoretical possibility of making carbon nanotubes based nanoelectronic devices with strong non-linear and multifunctional electronic properties is discussed in the report. It may be realised by joining nanotubes of different chiralities and consequently electronic characteristics (from typical semiconductors to semimetals, see for example [1]). Nanotubes of distinct radii and chiralities may be joined through a connecting surface representing a carbon structure packed by penta-, hexa- and heptagons [2].

In the literature [3] to analyse theoretically quantum current in two nanotube junction the direct diagonalization of electronic Hamiltonian of finite carbon cluster with junction structure containing 700 atoms is performed. Then the eigenvectors obtained are used to calculate the electric current under a voltage applied. Similar investigations of the current in three or more nanotubes junctions are absent in the literature. To investigate electric current in nanotube's junctions we use a phenomenological approach allowing analyse the current states in the nanotube junctions from known electron eigenfunctions of isolated nanotubes and presupposed nature of transition amplitude.

Let there are N single-layer and sufficiently long carbon nanotubes of different chiralities and radii connected between itself through transition surface area hereinafter named "connection area" (see Fig. 1). The transition amplitude between quantum states of different nanotubes is assumed to be small, that allows us to neglect the alternative electron transitions between chosen two states via interstitial ones. Hereinafter we denote the π-electron wave functions and quantum states energies of nanotube with number γ as $\mid k, m, n, \gamma\rangle$ and $E_{kmn\gamma}$ correspondingly, where $n = 1, 2$ is zone number in expression (1) for the signs $(-)$ and $(+)$. The π-electron states of the ideal nanotube are classified by two quantum numbers k, m, $\hbar k$ is the momentum of the electron along the axis of the cylinder, $\hbar m$ is the angular momentum, $\hbar$ is Planck's constant. The expressions for the π-electron wave functions of the ideal nanotube in tight-binding approximation may be found in our previous work [4], here we give only expression for the electron energy

$$\begin{aligned} E^{\pm}_{k,m} &= E_\pi \pm |\mathbf{H}_{01,k,m}| \\ \mathbf{H}_{01,k,m} &= \beta_0 + \exp(-im\varphi_2 - ikz_2)(\beta_1 + \beta_2 \exp(-im\varphi_1 - ikz_1), \end{aligned} \tag{1}$$

where E_π is the diagonal matrix element of the Hamiltonian, β_0, β_1, β_2 are the nonzero matrix elements based on the nearest neighbours atomic orbitals, the difference between the matrix elements depends on parameter a/R, where a is the nearest neighbour distance, R is nanotube's radius.

Apply at nanotube's ends electric potentials φ_γ, where $\gamma = 1, \ldots N$ (see Fig. 1), and suppose that the potentials in the nanotubes are constants, all voltage drop is only in the junction region. Transition matrix element $T^{k'm'n'\gamma'}_{kmn\gamma}$ between quantum states of different nanotubes $\mid k, m, n, \gamma\rangle$ and $|k', m', n', \gamma'\rangle$ (see Fig. 2) is assumed to be small. Suppose that quantum numbers correspond to electron moving to the contact, whereas k', m', n', γ' correspond to moving from the contact.

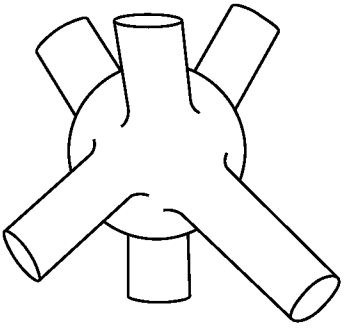

Fig. 1. Nanotube's contact area.

Using Fermi's formula for the transitions in the continuous spectra per unit time (see for example [5]) and taking into account multi-channel character of the electron transitions we obtain for the quantum current in the tube with number γ following expression

$$J_\gamma(\varphi_1 \ldots \varphi_2) \cong \frac{2\pi e}{\hbar} \int \sum_{m,n,m',n',\gamma'} \left| T^{k'm'n'\gamma'}_{kmn\gamma} \right|^2 D_{mn\gamma}(E + e\varphi_\gamma)$$
$$\times D_{m'n'\gamma'}(E + e\varphi_{\gamma'}) \left[f(E - \mu_\gamma + e\varphi_\gamma) - f(E - \mu_{\gamma'} + e\varphi_{\gamma'}) \right] dE \quad (2)$$

f is the Fermi–Dirac function, $D_{mn\gamma}(E)$ is partial electronic states density in the tube γ, equal to the number of states per unit energy interval on the equidistant line number m (see Fig. 2) with zone number n, e is the absolute value of electron charge. Function $D_{mn\gamma}(E)$ may have singularity at the energy E_{*m}, where the electron velocity along the tube axis become zero and partial density disconverges as $|E - E_{*m}|^{-1+1/2j}$, $j = 1, 2, 3, \ldots$. In expression (2) transitions between quantum states $|k, m, n, \gamma\rangle$ and $|k', m', n', \gamma'\rangle$ satisfy the energy conservation low $E_{kmn\gamma} + e\varphi_\gamma = E_{k'm'n'\gamma'} + e\varphi_{\gamma'}$; μ_γ is the chemical potential of isolated tube γ. For the ideal nanotubes the chemical potentials are the same and equal E_π, but in the case of doped or defective nanotubes are different.

The most simple analysis of the expression (2) may be performed for two nanotubes connection ($N = 2$). Supposing that chemical potentials of both tubes and potential φ_1 are zero, denoting the potential difference $\varphi_2 - \varphi_1$ through V, we obtain from (2) at zero temperature

$$J(V) \cong \frac{2\pi e}{\hbar} \int_0^{eV} \sum_{m,n,m',n'} \left| T^{k'm'n'2}_{kmn1} \right|^2 D_{mn1}(E) D_{m'n'2}(E + eV) dE. \quad (3)$$

Integral (3) may disconverge if singularities of functions $D_{mn1}(E)$ and $D_{m'n'2}(E + eV)$ coincide, that appear for discrete voltages with step of eV equal to energy distance

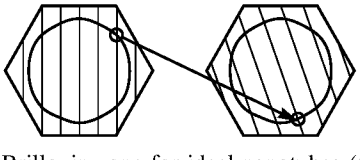

Fig. 2. Allowed states in the Brillouin zone for ideal nanotubes (6,0) and (6,2). The curves are level curves of the π-electron energy. The arrow denotes a quantum transition between nanotube's states.

$E_{*m'+1} - E_{*m'}$ between singularities of partial electron density function, depending on parameter a/R. More detailed analysis of the integral (3) disconvergency requires analytical investigation of the matrix element square dependence on the energy. If one of the joined tubes is metallic and the other has an energy gap then the current (3) is zero in the interval eV equal to the energy gap width. Change of the voltage sign leads to change of zone numbers of electron transition. The last may be cause of nonsymmetric current–voltage characteristic $I(V)$ because transition matrix element depends on the zone numbers the transition is realised between.

We discussed briefly peculiarities of two nanotubes junction current — voltage characteristic $I(V)$. In the many tube junction additive contributions from the different pairs of nanotubes make analysis of expression (2) more complicated, but nonmonotone dependence $I(V)$ in tubes, associated with electron states density singularities and presence of band gaps is summarised.

References

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